A CRITICAL ASSESSMENT OF THE SMAGORINSKY MODEL AND A NEW APPROACH TO LARGE-EDDY SIMULATIONS

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ABSTRACT

The Smagorinsky model for the large-eddy simulation of turbulence is critically assessed from a basic theoretical standpoint. It is shown that this model does not respond properly to the coarsening of the mesh because of its incorrect dependence on the dimensional mesh size. Rather, it is the dimensionless ratio of the computational mesh size to the Kolmogorov length scale that determines how well resolved a computation is and should be used to parameterize subgrid scale models. Furthermore, the Smagorinsky model has no dependence on rotational strains and depends improperly on the irrotational strain rate invariants. These facts tend to explain why the Smagorinsky constant is not in reality a constant in applications. An entirely new methodology for large-eddy simulations that is suitable for complex geometries is proposed that eliminates these deficiencies. In this new approach to large-eddy simulations, subgrid scale models go continuously to Reynolds stress models in the coarse mesh/infinite Reynolds number limit.

Key Words : Smagorinsky Model; Large-Eddy Simulations; Turbulence

1. INTRODUCTION

For the past thirty-five years, the Smagorinsky [1] model has served as a cornerstone for the large-eddy simulation (LES) of turbulence (see Rogallo and Moin [2] for an interesting review). Even though improvements have been attempted, the basic model has been largely maintained in applications. For example, the linear combination model of Bardina, Ferziger and Reynolds [3] introduced the scale similarity model for the subgrid scale Leonard and cross stresses but maintained the Smagorinsky model for the subgrid scale Reynolds stresses. Earlier investigators had modeled the subgrid scale Reynolds and cross stresses by the Smagorinsky model while the Leonard stresses were calculated directly by a convolution – an approach that destroyed the Galilean invariance of the filtered equations of motion (see Speziale [4] along with Biringen and Reynolds [5] and Moin and Kim [6]). The recently formulated dynamic subgrid scale stress model of Germano, Piomelli, Moin and Cabot [7] maintained the basic format of the Smagorinsky model. It merely allowed for the Smagorinsky constant to be a variable computed by an appeal to multiple filters (a test filter is introduced in addition to the grid filter). However, the Smagorinsky model suffers from a major deficiency in that it depends dimensionally on the computational mesh size. The quantity that determines how well resolved computations are is the ratio of the computational mesh size to the Kolmogorov length scale. In the Smagorinsky model, the subgrid scale stress $\tau_{ij} \to \infty$ as the mesh size $\Delta \to \infty$. Hence, a badly calibrated Reynolds stress model is obtained in the coarse mesh limit that is far too dissipative as will be discussed in this paper. Furthermore, the Smagorinsky model has no dependence on rotational strains which makes it impossible to describe rotating turbulent flows properly. The example of rotating isotropic turbulence will be considered to illustrate this point. In addition, its dependence on the irrotational strain rate invariants is incorrect – along with the improper dependence on the dimensional mesh size – necessitating, *ad hoc* adjustments of the Smagorinsky constant (the Smagorinsky constant can change by a factor of two even in basic flows). There is no question that there are problems with the Smagorinsky model and it should be abandoned in the future. It only correlates with DNS at the 50% level – an extremely poor result as will be demonstrated. The Smagorinsky model has probably only been successful because it drains approximately the correct amount of energy to account for the energy cascade to the scales that are left unresolved – a feature that is achieved by the *ad hoc* adjustment of the

Smagorinsky constant.

After first reviewing large-eddy simulations and the basic structure of the Smagorinsky model – which is nothing more than a tensorially invariant mixing length model where the mixing length is taken to be proportional to the computational mesh size – an entirely new methodology for large-eddy simulations will be presented. A grid function that depends on the ratio of the computational mesh size to the Kolmogorov length scale will be introduced that goes to one in the coarse mesh limit and vanishes in the fine mesh limit (in this way, one goes continuously from a DNS to an LES and then to a Reynolds-averaged Navier-Stokes (RANS) computation). Here, the Kolmogorov length scale is estimated by the Reynolds-averaged modeled dissipation rate equation. Since the turbulent dissipation rate is raised to the 1/4 power it only necessitates that the turbulent dissipation rate be calculated to within a 50% accuracy to get a good estimate of the Kolmogorov length scale as will be discussed. This is quite feasible with the current generation of Reynolds stress models for a broad range of flows. There is, additionally, a built-in dependence on rotational strains through anisotropic eddy viscosity terms which are dispersive and can account for backscatter effects. Furthermore, in the eddy viscosity there is is a dependence on both the irrotational and rotational strain rate invariants that is non-dimensional and is consistent with Reynolds stress models. Hence, a state-of-the-art Reynolds stress model is recovered in the coarse mesh/infinite-Reynolds-number limit; in the fine mesh limit, $\tau_{ij} \rightarrow 0$ yielding a direct numerical simulation (DNS). The approach to filtering will be discussed in considerable detail. A filter that yields the minimum contamination of the large scales is proposed in order to avoid the problem of defiltering which constitutes an ill-posed mathematical problem. In practical LES, the large-scale velocity field must be approximated by the filtered velocity. Reynolds-averaged quantities are then obtained by taking ensemble averages (time averages in a statistically steady turbulence). This new methodology for large-eddy simulations will be discussed which has the potential to bridge the gap between DNS, LES and RANS. It formally constitutes a combined LES/time-dependent RANS capability that requires doing a Reynolds stress calculation in parallel with the LES (this only adds approximately 10% to the computational expense). There is no question that the Smagorinsky model is deficient and should be abandoned as a relic of the past.

2. A CRITICAL REVIEW OF LARGE-EDDY SIMULATIONS AND THE SMAGORINSKY MODEL

The foundation was laid for the large-eddy simulation of turbulence in the ground breaking paper by Smagorinsky [1] over thirty years ago. Due to the fact that the small scales of turbulence serve mainly to drain energy from the large scales through the cascade process, it was felt that their effect could be modeled instead of being resolved. Since the small scales of turbulence were believed to be more universal in character based on theoretical considerations dating from the time of Kolmogorov [8], it was argued that the large scales – which contain most of the energy and are known to be affected significantly by the flow configuration under consideration – should be computed directly while the small scales are modeled. This has formed the basis for large-eddy simulations which were first implemented into meteorological computations shortly after the pioneering work of Smagorinsky [1].

Large-eddy simulations (LES) are based on the filtered equations of motion. Any flow variable ϕ, in the fluid domain D, can be decomposed into a large scale part and a small scale part, respectively, as follows [2]:

$$\phi = \overline{\phi} + \phi' \tag{1}$$

where

$$\overline{\phi} = \int_D G(\mathbf{x} - \mathbf{x}^*, \Delta)\phi(\mathbf{x}^*)d^3x^* \tag{2}$$

constitutes the spatial filter of ϕ. In (2), Δ is the computational mesh size and G is a filter function which is normalized as follows:

$$\int_D G(\mathbf{x} - \mathbf{x}^*, \Delta)d^3x^* = 1. \tag{3}$$

The filter function G has usually been taken to be a Gaussian filter in infinite domains or a piecewise continuous distribution of bounded support in compact domains (in the latter case, the simple box filter has been commonly used with finite difference methods; see Deardorff [9]). These features, along with the normalization constraint (3), guarantee that G becomes a Dirac delta sequence in the limit as $\Delta \to 0$:

$$\lim_{\Delta \to 0} \int_D G(\mathbf{x} - \mathbf{x}^*, \Delta)\phi(\mathbf{x}^*)d^3x^* = \int_D \delta(\mathbf{x} - \mathbf{x}^*)\phi(\mathbf{x}^*)d^3x^* \equiv \phi(\mathbf{x}) \tag{4}$$

where $\delta(\mathbf{x}-\mathbf{x}^*)$ is the Dirac delta function. Direct numerical simulations (DNS) are, thus, recovered in the fine mesh limit. Due to the Riemann-Lebesgue Theorem, (2) substantially reduces the amplitude of the high-wavenumber Fourier components in space of any flow variable ϕ (consequently, $\overline{\phi}$ represents the large scale part of ϕ). Unlike with traditional Reynolds averages,

$$\overline{\overline{\phi}} \neq \overline{\phi}, \quad \overline{\phi'} \neq 0 \tag{5}$$

in general.

In incompressible flows, a straightforward filtering of the Navier-Stokes equations yields [2]:

$$\frac{\partial \overline{u}_i}{\partial t} + \overline{u}_j \frac{\partial \overline{u}_i}{\partial x_j} = -\frac{\partial \overline{p}}{\partial x_i} + \nu \nabla^2 \overline{u}_i - \frac{\partial \tau_{ij}}{\partial x_j} \tag{6}$$

where $\overline{u}_i$ is the filtered velocity, $\overline{p}$ is the filtered kinematic pressure, ν is the kinematic viscosity and τ_{ij} is the subgrid scale stress tensor ($\tau_{ij} \to 0$ as $\Delta \to 0$). From the direct filtering of the continuity equation:

$$\frac{\partial \overline{u}_i}{\partial x_i} = 0. \tag{7}$$

The complete form of the subgrid scale stress tensor is as follows:

$$\tau_{ij} = L_{ij} + C_{ij} + R_{ij} \tag{8}$$

where

$$L_{ij} \equiv \overline{\overline{u}_i \overline{u}_j} - \overline{u}_i \overline{u}_j \tag{9}$$

$$C_{ij} \equiv \overline{\overline{u}_i u'_j + u'_i \overline{u}_j} \tag{10}$$

$$R_{ij} \equiv \overline{u'_i u'_j} \tag{11}$$

are, respectively, the Leonard stresses, subgrid scale cross stresses and subgrid scale Reynolds stresses (see Leonard [10]).

The first subgrid scale stress model was proposed by Smagorinsky [1] in his groundbreaking work on large-eddy simulations as discussed above. The Smagorinsky model constitutes an eddy viscosity model that takes the form:

$$\tau_{ij} = -C_s^2 \Delta^2 (2\overline{S}_{kl}\overline{S}_{kl})^{1/2} \overline{S}_{ij} \tag{12}$$

where

$$\overline{S}_{ij} = \frac{1}{2}\left(\frac{\partial \overline{u}_i}{\partial x_j} + \frac{\partial \overline{u}_j}{\partial x_i}\right)$$

is the filtered rate of strain tensor and C_s is a constant that bears his name (i.e., the Smagorinsky constant). Here, it should be noted that, for consistency, (12) only applies to the deviatoric, i.e., traceless, part of τ_{ij} (the isotropic part of τ_{ij} can be absorbed into the pressure in incompressible flows).

For thin shear flows where $\overline{\mathbf{u}} = \overline{u}(y)\,\mathbf{i}$ (given that $\mathbf{i}$ is a unit vector in the x-direction) it follows that the Smagorinsky model (12) collapses to the form

$$\tau_{xy} = -\frac{1}{2}C_s^2\Delta^2\left|\frac{d\overline{u}}{dy}\right|\frac{d\overline{u}}{dy} \tag{13}$$

which is identical in form to the mixing length theory of Prandtl [11] for the Reynolds shear stress where the mixing length is proportional to the computational mesh size Δ. Hence, it can be argued that the Smagorinsky model is nothing more than a tensorially invariant mixing length theory where the mixing length is taken to be proportional to the computational mesh size since it is a subgrid scale stress model rather than a Reynolds stress model.

The Smagorinsky model has several deficiencies that can be summarized as follows:

(1) The Smagorinsky constant is not in reality a constant. It can vary by as much as a factor of two or three from flow to flow. This is because the Smagorinsky model is badly parameterized. Furthermore, it only correlates with DNS at the 50% level. To get an idea of how poor this result is, the correlation between the functions $y = x$ and $y = e^{-x}$ on the interval [0, 1] is more than 50% despite the fact that they are qualitatively different functions (one is monotonically increasing while the other is monotonically decreasing)!

(2) The Smagorinsky model *does not* depend on the rotational strains through the invariant $\xi \propto (\overline{W}_{ij}\overline{W}_{ij})^{1/2}$ ($\overline{W}_{ij} \equiv \frac{1}{2}(\partial\overline{u}_i/\partial x_j - \partial\overline{u}_j/\partial x_i)$ is the filtered vorticity tensor) and, furthermore, has the wrong dependence on the irrotational strain rate invariant $\eta \propto (\overline{S}_{ij}\overline{S}_{ij})^{1/2}$. For Reynolds stress models in equilibrium, the eddy viscosity

$$\nu_T \propto \frac{3}{3 - 2\eta^2 + 6\xi^2}$$

(see Gatski and Speziale [12]).

(3) The dependence on the computational mesh size Δ should be through the dimensionless ratio Δ/L_K. *What determines how well a computation is resolved is whether or not*

the grid size is small (or large) compared to the Kolmogorov length scale. The dimensional dependence on Δ in the Smagorinsky model is simply incorrect. In the Smagorinsky model, $\tau_{ij} \to \infty$ as $\Delta \to \infty$. Hence, a badly calibrated Reynolds stress model is obtained in the coarse mesh limit. The model becomes far too dissipative as the mesh becomes coarse.

In so far as point (2) is concerned, this makes it impossible for the Smagorinsky model to properly describe rotating flows. For example, it is well known that in a rapidly rotating isotropic turbulence, the cascade is essentially shut off so that the turbulence undergoes a linearly viscous decay (see Speziale, Mansour and Rogallo [13]). Hence, it is possible to conduct direct simulations even at high turbulence Reynolds numbers. The Smagorinsky model is far too dissipative in this case where it can yield results that are completely erroneous. For a rapidly rotating isotropic turbulence, the Smagorinsky constant is essentially zero except, perhaps, at astronomically high Reynolds numbers or for extremely coarse meshes.

While the dynamic subgrid scale model of Germano, Piomelli, Moin and Cabot [7] does address point (1) through a variable Smagorinsky constant, it does not address the other criticisms. Furthermore, with its multiple filters it is not suitable for complex geometries. If LES is to make an impact on the complex turbulent flows of technological importance it is essential that this shotcoming be overcome. In the next section, a new approach to large-eddy simulations will be proposed that overcomes each of the deficiencies of the Smagorinsky model outlined above.

3. A NEW APPROACH TO LARGE-EDDY SIMULATIONS

The new methodology that is being proposed for large-eddy simulations has subgrid scale stress models that are of the following form:

$$\tau_{ij} = -[1 - exp(-\beta\Delta/L_K)]^n \alpha_1 f(\eta,\xi)\frac{K^2}{\varepsilon}\overline{S}_{ij} + \tau_{ij}^A \tag{14}$$

where τ_{ij}^A represents the anisotropic part of the subgrid scale stress tensor. Here, an overbar represents a *standard* filter whereas

$$\eta = \alpha_2(\overline{S}_{ij}\overline{S}_{ij})^{1/2}\frac{K}{\varepsilon}, \quad \xi = \alpha_3(\overline{W}_{ij}\overline{W}_{ij})^{1/2}\frac{K}{\varepsilon} \tag{15}$$

where $\overline{S}_{ij}$ and $\overline{W}_{ij}$ are the filtered rate of strain and vorticity tensors, Δ is the computational mesh size, $L_K \equiv \nu^{3/4}/\varepsilon^{1/4}$ is the Kolmogorov length scale, and β, α_1, α_2 and α_3 are constants; α_1, α_2 and α_3 are obtained from a Reynolds stress model along with the function f). Here, K and ε represent the Reynolds-averaged turbulent kinetic energy and dissipation rate obtained from a *Reynolds stress calculation* with the two-equation models equivalent to that given above in the coarse mesh limit as $\Delta/L_K \to \infty$.

In the coarse mesh limit, a Reynolds stress model given by

$$R_{ij} = -\alpha_1 f(\eta,\xi)\frac{K^2}{\varepsilon}\overline{S}_{ij} + R_{ij}^A \tag{16}$$

is recovered which is an explicit algebraic stress model (see Gatski and Speziale [12]). The turbulent dissipation rate ε – and, hence, the turbulent kinetic energy K – have to be obtained anyway in order to get an estimate of the Kolmogorov length scale L_K. Since, the Kolmogorov length scale $L_K = \nu^{3/4}/\varepsilon^{1/4}$, the dissipation rate only has to be estimated to within 50% with the modeled dissipation rate equation to get a good estimate of the Kolmogorov length scale (the dissipation rate is raised to the 1/4 power as mentioned before). This is quite feasible with state-of-the-art Reynolds stress models. Thus, this methodology requires that a RANS calculation be done in parallel with the LES. This will, in most circumstances, only add at most 10% to the computational expense. Here, we parameterize the model in terms of the Reynolds-averaged turbulent kinetic energy and dissipation since the subgrid scale turbulent kinetic energy and dissipation rate can vary too much locally. This model has been written before in the shorthand notation as (see Speziale [14])

$$\tau_{ij} = [1 - exp(-\beta\Delta/L_K)]^n R_{ij} \tag{17}$$

where R_{ij} is a Reynolds stress model that is written partially in terms of filtered fields. An explicit algebraic stress model is used for this purpose as discussed above.

The anisotropic eddy viscosity terms take the form

$$\tau_{ij}^A = [1 - exp(-\beta\Delta/L_K)][\alpha_4 \frac{K^3}{\varepsilon^2} f(\eta,\xi)(\overline{W}_{ik}\overline{S}_{kj} + \overline{W}_{jk}\overline{S}_{ki})$$

$$+\alpha_5 f(\eta,\xi)\frac{K^3}{\varepsilon^2}(\overline{S}_{ik}\overline{S}_{kj} - \frac{1}{3}\overline{S}_{kl}\overline{S}_{kl}\delta_{ij})] \tag{18}$$

where again the overbar represents a filtered quantity whereas K and ε are the Reynolds-averaged turbulent kinetic energy and dissipation rate obtained from a Reynolds stress calculation (α_4 and α_5 are constants). In the coarse mesh limit as $\Delta/L_K \to \infty$, the anisotropic eddy viscosity terms of an explicit algebraic stress model are recovered (see Gatski and Speziale [12]). These terms are dispersive in character and can account for backscatter effects. For example, Clark, Ferziger and Reynolds [15] obtained the subgid scale stress model from a Taylor expansion:

$$\tau_{ij} = -C_s^2\Delta^2(2\overline{S}_{kl}\overline{S}_{kl})^{1/2}\overline{S}_{ij} + \frac{1}{12}\Delta^2\frac{\partial\overline{u}_i}{\partial x_k}\frac{\partial\overline{u}_j}{\partial x_k}. \tag{19}$$

Since

$$\frac{\partial\overline{u}_i}{\partial x_j} = \overline{S}_{ij} + \overline{W}_{ij} \tag{20}$$

it is a simple matter to show that (19) is of the same tensorial form as (18). However, it depends improperly on the dimensional mesh size and dimensional strain rate invariants (the term containing $\overline{W}_{ik}\overline{W}_{kj}$ was, furthermore, shown by Speziale [16] to be inadmissible for Reynolds stress models). It was shown by Clark, Ferziger and Reynolds [15] that this kind of anisotropic eddy viscosity term can account for backscatter effects.

For Reynolds stress models in equilibrium

$$f(\eta,\xi) = \frac{3}{3 - 2\eta^2 + 6\xi^2}. \tag{21}$$

A singularity can occur when this expression is applied to turbulent flows where there are significant departures from equilibrium. Gatski and Seziale [12] intoduced the simple regularization

$$\frac{3}{3 - 2\eta^2 + 6\xi^2} \approx \frac{3(1+\eta^2)}{3 + \eta^2 + 6\xi^2\eta^2 + 6\xi^2} \tag{22}$$

which is obtained by a Taylor series expansion. For turbulent flows in equilibrium where $\eta, \xi < 1$, it yields results that are indistinguishable from (21) where it formally applies. But it is regular and computable for *all* values of η and ξ. More recently, Speziale and Xu [17] obtained expressions via a formal Pade$'$ approximation that builds in some limited agreement with the Rapid Distortion Theory (RDT) theory solutions for plane shear and plane strain turbulence. The constants in this Reynolds stress model are given by

$$\alpha_1 = 0.374, \quad \alpha_2 = 0.145, \quad \alpha_3 = 0.308, \tag{23}$$

$$\alpha_4 = 0.115, \quad \alpha_5 = 0.108. \tag{24}$$

This Reynolds stress model has been tested in a variety of benchmark turbulent flows (see Gatski and Speziale [12]). The turbulent kinetic energy K and dissipation rate ε are obtained from modeled versions of their Reynolds-averaged transport equations which take the form (cf. Speziale [16])

$$\frac{\partial K}{\partial t} + \overline{\mathbf{u}} \cdot \nabla K = \mathcal{P} - \varepsilon + \frac{\partial}{\partial x_i}\left(\frac{\nu_T}{\sigma_k}\frac{\partial K}{\partial x_i}\right) \tag{25}$$

$$\frac{\partial \varepsilon}{\partial t} + \overline{\mathbf{u}} \cdot \nabla \varepsilon = C_{\varepsilon 1}\frac{\varepsilon}{K}\mathcal{P} - C_{\varepsilon 2}\frac{\varepsilon^2}{K} + \frac{\partial}{\partial x_i}\left(\frac{\nu_T}{\sigma_\varepsilon}\frac{\partial \varepsilon}{\partial x_i}\right) \tag{26}$$

where $\mathcal{P} \equiv -\tau_{ij}\partial\overline{u}_i/\partial x_j$ is the turbulence production and $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, σ_k and σ_ε are constants that assume the values of 1.44, 1.83, 1.0 and 1.3, respectively. These equations have served as a cornerstone for two-equation models. In order to integrate this model to a wall it is only necessary to remove the singularity in the destruction term that appears on the right-hand-side of (26) with the coefficient $C_{\varepsilon 2}$ (see Speziale and Abid [18]). *No ad hoc wall damping functions are needed in the Reynolds stress model.* This is accomplished by replacing $C_{\varepsilon 2}$ with the term

$$C_{\varepsilon 2}[1 - exp(-R_y/10)] \tag{27}$$

where $R_y = K^{1/2}y/\nu$ given that ν is the kinematic viscosity and y is the coordinate normal to the wall. In many applications, a small vortex stretching term has been added to (26) to make the calculations better behaved. It removes the singularity in plane stagnation point turbulent flows and, furthermore, allows for the description of both the log-layer and homogeneous turbulence in equilibrium with a simple unified model where it is not necessary to solve the cubic equation arising out of the consisistency condition (see Abid and Speziale [19] and Speziale, Jongen and Gatski [20]).

In a rapidly rotating isotropic turbulence, $f(\eta, \xi) \to 0$ so $\tau_{ij} \to 0$ yielding a DNS. This results from the fact that [16]

$$\overline{W}_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i}\right) + e_{mji}\Omega_m$$

in rotating frames where Ω_m is the rotation rate of the frame and e_{mji} is the permutation tensor (hence, $\xi \sim \Omega$ in a rapidly rotating flow with angular velocity Ω). As mentioned earlier, in a rapidly rotating isotropic turbulence the energy cascade is essentially shut off so that direct numerical simulations can be conducted with a 128^3 mesh even at high turbulence Reynolds numbers. A 128^3 mesh forms a cornerstone of this new approach to LES as will soon be discussed. In contrast, the Smagorinsky model is far too dissipative so it yields incorrect results for this problem.

The grid function

$$[1 - exp(-\beta\Delta/L_K)]^n \tag{28}$$

bridges the gap between DNS, LES and RANS where L_K is the Kolmogorov length scale $L_K = \nu^{3/4}/\varepsilon^{1/4}$ estimated from a Reynolds stress calculation (again, Δ is the computational mesh size). In the limit as $\Delta/L_K \to \infty$ the grid function goes to one and we recover a Reynolds stress model whereas in the limit as $\Delta/L_K \to 0$, it goes to zero and we formally recover a DNS. Actually, when Δ/L_K is of order one, we should have a DNS (this has been built into the calibration). Since $L_K \equiv R_t{}^{-3/4}K^{3/2}/\varepsilon$ where $R_t \equiv K^2/\nu\varepsilon$ is the turbulence Reynolds number, $\Delta/L_K \to \infty$ as $R_t \to \infty$ (thus, we recover a Reynolds stress model in the coarse mesh/infinite-Reynolds-number limit). For the initial calculations, n has been taken to be one and β has been calibrated as follows:

$$\beta \approx 0.001. \tag{29}$$

A power law for the grid function has been theoretically obtained using Renormalization Group methods (Woodruff and Hussaini [21]). Note that for $\Delta/L_K < 100$, we approximately obtain a power law from (28) via a Taylor expansion. Most practical LES are conducted for $\Delta/L_K = 10 - 100$. In complex geometries,

$$\Delta = (\Delta_x\Delta_y\Delta_z)^{1/3} \tag{30}$$

where Δ_x, Δ_y and Δ_z are the mesh sizes in the x, y and z directions, respectively, obtained after a coordinate transformation. The box filter can be used in complex geometries which is given by

$$G(\mathbf{x}-\mathbf{x}^*,\Delta) = \begin{cases} 1/8\Delta^3, & |x_i - x_i^*| \le \Delta_{x_i} \\ 0, & |x_i - x_i^*| > \Delta_{x_i} \end{cases} \tag{31}$$

for $i = 1,2,3$ where Δ_{x_i}, is Δ_x, Δ_y and Δ_z, respectively (Δ is given by (30)).

Finally, some comments are needed concerning the choice of a filter in this new approach to large-eddy simulations and the melding together of spatial filtering in LES and Reynolds averaging in RANS. We want a filter that yields the minimum contamination of the large scales. The reason for this is clear; defiltering must be avoided since it constitutes an ill-posed mathematical problem as stated earlier. The purpose of practical LES is to predict the Reynolds-averaged fields. In order to do so, the filtered velocity, which is calculated, must invariably be used to estimate the large-scale part of the instantaneous velocity which then yields the Reynolds-averaged fields through appropriate ensemble or time averages. The filtered equations of motion (6) are of the same form as the Reynolds-averaged equations. In the coarse mesh limit the ramp function will be one and the model will be so dissipative that a RANS calculation will be recovered with a state-of-the-art Reynolds stress model. It is envisoned that ensemble averages will be taken even if we are conducting a time-dependent RANS. Thus, we do not need to know the effect of the filter – which can never be fully known in complex geometries – except, perhaps for model calibration in benchmark flows. This allows us to meld together the LES and RANS methodologies which are normally treated as disparate approaches. In both of these approaches we calculate what is tantamount to the large-scale velocity field – through the same basic equations of motion – and then obtain the Reynolds-averaged fields through ensemble averages. The large scales make the dominant contribution to the most pertinent fields such as the turbulent kinetic energy. A minimum contamination of the large scales can be accomplished with, of the order of, a 128^3 computational mesh using a filter with a compact support – such as the box filter – which has a small filter width of, say, two mesh points. Some of the previously conducted coarse grid LES (which has typically had no more than 32^3 mesh points) must be avoided wherein the filter width has, at times, been as much as 25% of the computational domain, significantly contaminating the large scales. Besides, recent increases in computational capacity have begun to make 128^3 computations much more feasible for engineering calculations (a small compromise to 100^3 computations can always be made). In addition, it should be noted that practical LES – in complex geometries – will require the use of finite difference techniques with a compact filter where we will never make explicit use of the filter (these finite difference methods should, furthermore, be based on fourth-order accurate finite difference schemes for better accuracy).

4. CONCLUSIONS

The Smagorinsky model for large-eddy simulations in turbulence was critically reviewed and a new approach to large-eddy simulations was presented. The following conclusions were arrived at:

(1) The Smagorinsky constant is not in reality a constant. It can vary by as much as a factor of two or three from flow to flow because the model is badly parameterized. In the new approach to LES, this variation is parameterized by the Reynolds-averaged turbulent kinetic energy and dissipation rate that are obtained from a RANS calculation which is done in parallel with the LES adding only approximately 10% to the computational expense. These are needed anyhow to get an estimate of the Kolmogorov length scale which is an integral part of the new methodology. We decidedly *do not* use the subgrid scale turbulent kinetic energy and dissipation rate for this purpose since they can vary too much. The variation of the constants can probably be adequately parameterized by the mean turbulent fields K and ε.

(2) The Smagorinsky model *does not* depend on rotational strains and, furthermore, has the wrong dependence on the irrotational strain rate invariant. For Reynolds stress models in equilibrium,

$$f(\eta,\xi) = \frac{3}{3 - 2\eta^2 + 6\xi^2}$$

(regularized versions of this representation that avoids the singularity have been used). The choice of $f(\eta,\xi) \propto \eta$ in the Smagorinsky model is simply wrong and probably contributes to the Smagorinsky constant changing so much. Furthermore, an additional dependence on rotational strains has been built in through anisotropic eddy viscosity terms which are dispersive and account for backscatter effects. The strain-dependence through the function $f(\eta,\xi)$ makes it possible to properly describe rotating turbulent flows (the example of rotating isotropic turbulence was presented) and, also, allows for the integration of the model to solid boundaries with no wall damping. The Smagorinsky model, on the other hand, decidedly needs empirical wall damping.

(3) The dependence on the computational mesh size Δ in the new approach to LES is through the dimensionless ratio Δ/L_K. *What determines how well a computation is resolved is whether or not the grid size is small (or large) compared to the Kolmogorov length scale.*

The dimensional dependence on Δ in the Smagorinsky model is simply incorrect. Since a filter is used that yields a minimum contamination of the large scales (this is guaranteed by any filter with a small compact support on a 128^3 mesh), a state-of-the-art Reynolds stress model is recovered in the coarse mesh/infinite Reynolds number limit as Δ/L_K tends to infinity ($L_K \equiv R_t{}^{-3/4}K^{3/2}/\varepsilon$ where R_t is the turbulence Reynolds number). On the other hand, the Smagorinsky model goes to a badly calibrated Reynolds stress model in the coarse mesh limit that is far too dissipative (the same is true of the dynamic subgrid scale model).

Hence, with this new methodology it is possible to achieve the long held dream of going continuously from a large-eddy simulation to a Reynolds stress calculation as the mesh becomes coarse or the Reynolds number becomes extremely large. In wall-bounded geometries, the best we can currently do – at extremely high Reynolds numbers – is a Reynolds stress calculation since the crucial wall-layer is not resolved. Of course, as with the Smagorinsky model, the subgrid scale stress $\tau_{ij} \to 0$ in the new model as $\Delta \to 0$ allowing a DNS to be recovered. However, here the dependence is properly parameterized by the dimensionless ratio of the computational mesh size to the Kolmogorov length scale, Δ/L_K.

Some final comments are in order concerning the role of direct and large-eddy simulations in turbulence. There is no question that DNS – and the computer in general – has revolutionized the study of turbulence. DNS has already shed new light on the physics of a range of basic turbulent flows and the future potential is enormous. It already appears that in the not too distant future, DNS will entirely replace basic benchmark physical experiments for homogeneous turbulence and near-wall turbulent flows, at lower turbulence Reynolds numbers. However, it appears that DNS will, for a long time to come, be limited to relatively simple geometries and low to moderate turbulence Reynolds numbers. Direct simulations of the kind of complex turbulent flows of technological importance, at high turbulence Reynolds numbers, could require the generation of data bases with upwards of 10^{20} numbers. Thus, it is crucial that large-eddy simulations be made to work. As far as LES is concerned, it must be said that it has never lived up to its initial promise. The way that traditional LES has been formulated is probably only suitable for doing less expensive parametric studies of benchmark direct simulations once the reliability of the subgrid scale model has been established by DNS for the baseline case. In order to solve the complex turbulent flows of technological importance, an entirely new approach to LES is needed. Prandtl's mixing length theory was abandoned after four decades when it became apparent that it could not address complex turbulent flows. It is time that the same be done with the Smagorinsky model in favor of a new approach to LES.

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REFERENCES

1. J. Smagorinsky, "General circulation experiments with the primitive equations," *Mon. Weather Review* **91**, 99-165 (1963).

2. R. S. Rogallo and P. Moin, "Numerical simulation of turbulent flows," *Ann. Rev. Fluid Mech.* **16**, 99-137 (1984).

3. J. Bardina, J. H. Ferziger and W. C.Reynolds, "Improved turbulence models based on large-eddy simulation of homogeneous, incompressible turbulent flows," *Stanford University Technical Report No. TF-19* (1983).

4. C. G. Speziale, "Galilean invariance of subgrid scale models in the large-eddy simulation of turbulence," *J. Fluid Mech.* **156**, 55-62 (1985).

5. S. Biringen and W. C. Reynolds, "Large-eddy simulation of the shear free turbulent boundary layer," *J. Fluid. Mech.* **103**, 53-63 (1981).

6. P. Moin, and J. Kim, "Numerical investigation of turbulent channel flow," *J. Fluid. Mech.* **118**, 341-377 (1982).

7. M. Germano, U. Piomelli, P. Moin, and W. H. Cabot, "A dynamic subgrid-scale eddy viscosity model," *Phys. Fluids* **3**, 1760-1765 (1991).

8. A. N. Kolmogorov, "The equations of turbulent motion in an incompressible fluid," *Izv. Acad. Sci. USSR, Phys.* **6**, 56-58 (1942).

9. J. W. Deardorff, "A numerical study of three-dimensional turbulent channel flow at large Reynolds numbers," *J. Fluid. Mech.* **41**, 453-480 (1970).

10. A. Leonard, "On the energy cascade in large-eddy simulations of turbulent flows," *Adv. Geophys. A* **18**, 237-248 (1974).

11. L. Prandtl, "Über die ausgebildete turbulenz," *ZAMM* **5**, 136-139 (1925).

12. T. B. Gatski and C. G. Speziale, "On explicit algebraic stress models for complex turbulent flows," *J. Fluid Mech.* **254**, 59-78 (1993).

13. C. G. Speziale, N. N. Mansour and R. S. Rogallo, "The decay of isotropic turbulence in a rapidly rotating frame," in *Studying Turbulence Using Numerical Simulation Databases,*

(P. Moin, W. C. Reynolds and J. Kim, eds.) pp. 205-211, NASA Ames – Stanford Center for Turbulence Research (1987).

14. C. G. Speziale, "Computing Non-Equilibrium Turbulent Flows with Time-Dependent RANS and VLES," *Lecture Notes in Physics* **490**, pp. 123-129, Springer-Verlag (1997).

15. R. A. Clark, J. H. Ferziger and W. C. Reynolds, "Evaluation of subgrid-scale models using an accurately simulated turbulent flow," *J. Fluid. Mech.* **91**, 1-16 (1979).

16. C. G. Speziale, "Modeling of Turbulent Transport Equations," in *Simulation and Modeling of Turbulent Flows*, (T. B. Gatski, M. Y. Hussaini and J. L. Lumley, eds.), pp. 185-242, Oxford Univ. Press, New York (1996).

17. C. G. Speziale and X. H. Xu, "Towards the development of second-order closure models for non-equilibrium turbulent flows," *Int. J. Heat & Fluid Flow* **17**, 238-244 (1996).

18. C. G. Speziale and R. Abid, "Near-wall integration of Reynolds stress turbulence closures with no wall damping," *AIAA J.* **33**, 1974-1977 (1995).

19. R. Abid and C. G. Speziale, "The freestream matching condition for stagnation point turbulent flows: An alternative formulation," *ASME J. Appl. Mech.* **63**, 95-100 (1996).

20. C. G. Speziale, T. Jongen and T. B. Gatski, "On a unified equilibrium hypothesis for algebraic stress models of turbulence," *Boston University Technical Report No. AM-97-026* (1997).

21. S. Woodruff and M. Y. Hussaini, *Private Communication* (1996).